

AD-A134 008

THEORETICAL STUDIES IN MOLECULAR FRAGMENTATION:
PROCESSES, ENERGIES AND DIAGNOSTICS(U) SMITHSONIAN
ASTROPHYSICAL OBSERVATORY CAMBRIDGE MA K P KIRBY
22 SEP 83 N00014-82-K-0536

1/1

UNCLASSIFIED

F/G 7/4

NL

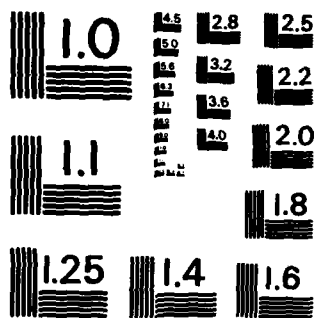
END

DATE

FILED

*1

OTIC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS - 1963 - A

10-9134-000

1. TITLE RESEARCH IN PHYSICS OF PLASMA	
2. AUTHOR(S) WILLIAM F. FLYNN	
3. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) SAATCHIAN Astrophysical Observatory 60 Garden Street Cambridge, MA 02138	
4. AUTHOR(S) WILLIAM F. FLYNN	
5. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Office of Naval Research 800 N. Quincy Avenue Arlington, Virginia 22217	
6. DATE OF REPORT October 22, 1968	
7. DATE OF PUBLICATION 1968	
8. DISTRIBUTION STATEMENT (of this report) Approved for public release; distribution unlimited.	
9. DISTRIBUTION STATEMENT (of the abstract appearing in this report) Approved for public release; distribution unlimited.	
10. SUPPLEMENTARY NOTES	
11. ABSTRACT (Maximum length 200 words) Abstracting this report is permitted; reproduction is prohibited.	
12. KEYWORDS Plasma; Physics; Research	

DTIC
ELECTE
OCT 24 1968
S D

CONT'D
20.

on the excited electronic states of NH_3 .

THEORETICAL STUDIES IN MOLECULAR FRAGMENTATION:

PROCESSES, ENERGETICS AND DIAGNOSTICS

Contract NO0014-82-K-0536

Annual Report

For the period 1 September 1982 through 31 August 1983

Principal Investigator

Dr. Kate P. Kirby

Prepared for

Office of Naval Research
Arlington, Virginia 22217

September, 1983

Smithsonian Institution
Astrophysical Observatory
Cambridge, Massachusetts 02138

Accession For	
NTIS GRA&I	<input checked="checked" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By _____	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A	



The Smithsonian Astrophysical Observatory
is a member of the
Harvard Smithsonian Center for Astrophysics

The ONR Technical Officer for this grant is Dr. Bobby R. Junker, Code 421,
Office of Naval Research, 800 N. Quincy Avenue, Arlington, Virginia 22217
Reproduction in whole or in part is permitted for any purpose of the
United States Government.

THEORETICAL STUDIES IN MOLECULAR FRAGMENTATION:

PROCESSES, ENERGETICS AND DIAGNOSTICS

Annual Progress Report

For the period 1 September 1982 through 31 August 1983

Principal Investigator

Dr. Kate P. Kirby

Our research is directed toward providing diagnostic tools with which to identify and quantify the presence of fragment species and their energy states resulting from molecular destruction processes. The necessary diagnostics data base for small diatomic fragments such as CO, NH, and CN includes potential energy curves, particularly excited electronic states, and transition probabilities. We are using theoretical ab initio methods to calculate the molecular structure and properties of the low-lying 1Π and $1\Sigma^+$ states of CO. In addition, we have used spectroscopic information as well as the theoretical dipole moment of CN, to calculate vibration-rotation transition probabilities and lifetimes for vibrationally hot CN. A postdoctoral research fellow, Dr. Evelyn Goldfield, has been hired, and is currently commencing work on the excited states of NH.

Dr. David L. Cooper and I have recently devised a set of calculations for the $1\Sigma^+$ and 1Π manifolds of CO which appears to be very promising. We construct large-scale configuration interaction (CI) wavefunctions (47,036 and 26,951 configurations for the 1Π and $1\Sigma^+$ states, respectively) which include both valence and Rydberg mixing so that the molecular bonding

regions as well as the atomic asymptotic limits are accurately described. A new set of ALCHEMY programs has been obtained which uses the symbolic matrix method (Liu and Yoshimine, J. Chem. Phys. 74, 612 (1981)), in addition to a direct CI method and has the capabilities needed to obtain efficiently the potential energies for wavefunctions with large numbers of configurations. So far, our calculations give energy splittings in excellent agreement with available spectroscopic data for the known excited $B^1\Sigma^+$ and $E^1\Pi$ states, both of which have some Rydberg character at small internuclear separations R , and at large R dissociate to ground state atoms. We anticipate that we will also be able to characterize the new $D^1\Sigma^+$ state which has recently been identified from laser-induced fluorescence studies (G.L. Wolk and J.W. Rich, J. Chem. Phys. 79, 12. (1983)). The transition moments obtained from our preliminary calculations on the $X^1\Sigma^+ - A^1\Pi$ system have been shown to be in excellent agreement with experimental measurements (R.W. Field et al., J. Chem. Phys. 78, 2838 (1983)).

END

DATE
FILMED

11 - 83

DTIC